

POOL License

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POOL is a suite of programs for protein loop backbone structure determination from residual dipolar couplings (RDCs) (only two RDCs per residue are required) in one alignment medium. Additional experimental data, e.g., TALOS dihedral restraints and unambiguous backbone NOEs can be used to filter the candidate loop conformations. POOL is a part of RDC-ANALYTIC suite of programs for high-resolution protein backbone fold determination from RDCs. RDC-ANALYTIC/POOL is developed in the lab of Prof. Bruce R. Donald at Duke University.

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Contact Info:

Bruce R. Donald
Duke University
Department of Computer Science
Levine Science Research Center (LSRC)
Durham, NC 27708-0129
USA
email: www.cs.duke.edu/brd/

<signature of Bruce Donald>, August 04, 2012
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- [1] Chittaranjan Tripathy, Jianyang Zeng, Pei Zhou, and Bruce Randall Donald. Protein loop closure using orientational restraints from NMR data. *Proteins: Structure, Function, and Bioinformatics*, 80(2):433–453, 2012.
- [2] Chittaranjan Tripathy, Jianyang Zeng, Pei Zhou, and Bruce Randall Donald. Protein loop closure using orientational restraints from NMR data. In Vineet Bafna and S. Sahinalp, editors, *Proceedings of the 15th Annual International Conference on Research in Computational Molecular Biology (RECOMB), Vancouver, BC Canada*, volume 6577 of *Lecture Notes in Computer Science*, pages 483–498. Springer Berlin / Heidelberg, 2011.
- [3] Anna Yershova, Chittaranjan Tripathy, Pei Zhou, and Bruce Randall Donald. Algorithms and Analytic Solutions using Sparse Residual Dipolar Couplings for High-Resolution Automated Protein Backbone Structure Determination by NMR. *The Ninth International Workshop on the Algorithmic Foundations of Robotics (WAFR)*, 68:355–372, 2010.
- [4] Jianyang Zeng, Jeffrey Boyles, Chittaranjan Tripathy, Lincong Wang, Anthony Yan, Pei Zhou, and Bruce Randall Donald. High-resolution protein structure determination starting with a global fold calculated from exact solutions to the RDC equations. *Journal of Biomolecular NMR*, 45(3):265–281, 2009.
- [5] Bruce R. Donald and Jeffrey Martin. Automated NMR Assignment and Protein Structure Determination using Sparse Dipolar Coupling Constraints. *Progress in Nuclear Magnetic Resonance Spectroscopy*, 55(2):101–127, 2009.
- [6] Lincong Wang, Ramgopal R. Mettu, and Bruce R. Donald. A Polynomial-Time Algorithm for *De Novo* Protein Backbone Structure Determination from NMR Data. *Journal of Computational Biology*, 13(7):1276–1288, 2006.
- [7] Lincong Wang and Bruce Randall Donald. Analysis of a Systematic Search-Based Algorithm for Determining Protein Backbone Structure from a Minimal Number of Residual Dipolar Couplings. In *Proceedings of the 2004 IEEE Computational Systems Bioinformatics Conference (CSB04), Stanford CA*, pages 319–330, 2004.

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```
<program> Copyright (C) <year> <name of author>
```

```
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```

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